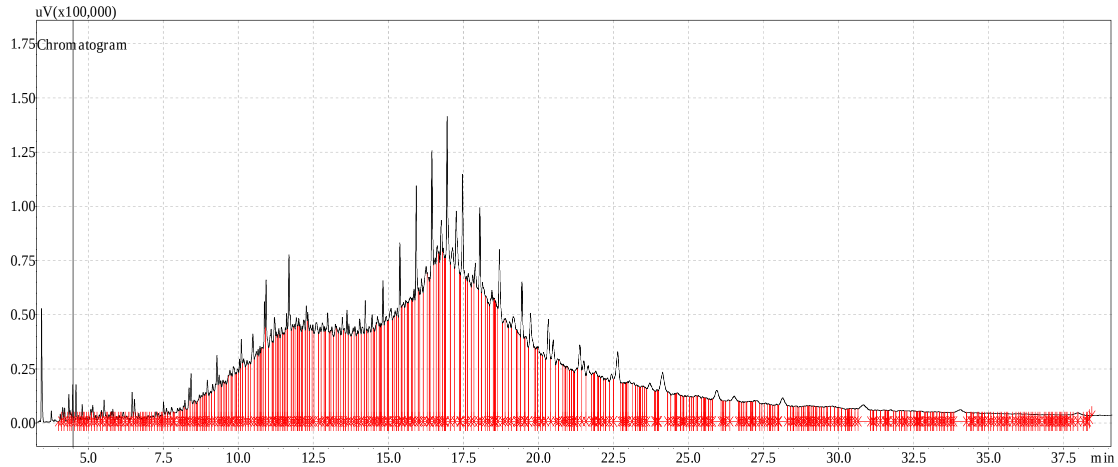
Development of a novel direct-infusion atmospheric pressure chemical ionization mass spectrometry method for the analysis of heavy hydrocarbons in light shredder waste

Nadim Hourani, Nikolai Kuhnert*

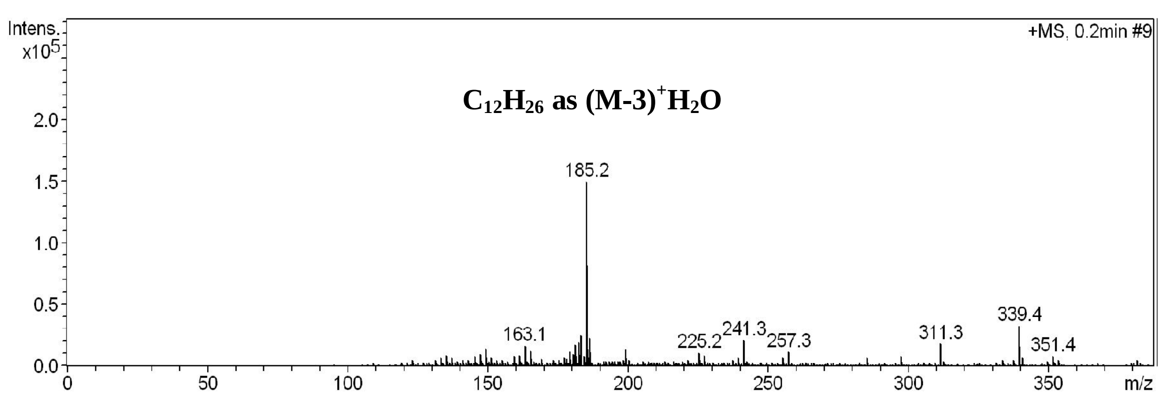
School of Engineering and Science, Jacobs University Bremen, P.O. Box 750 561, 28725 Bremen, Germany, Fax: +49 421 200 3229; Tel: +49 421 200 3120; E-mail*: *n.kuhnert@jacobs-university.de

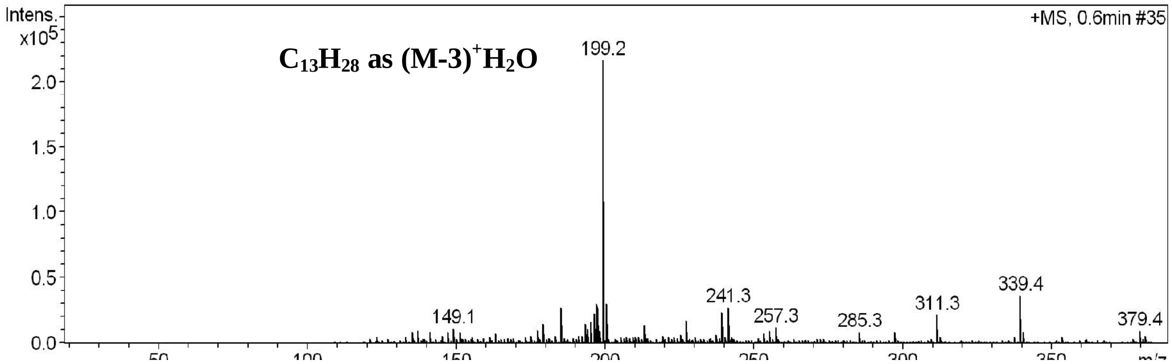
Supplementary Information

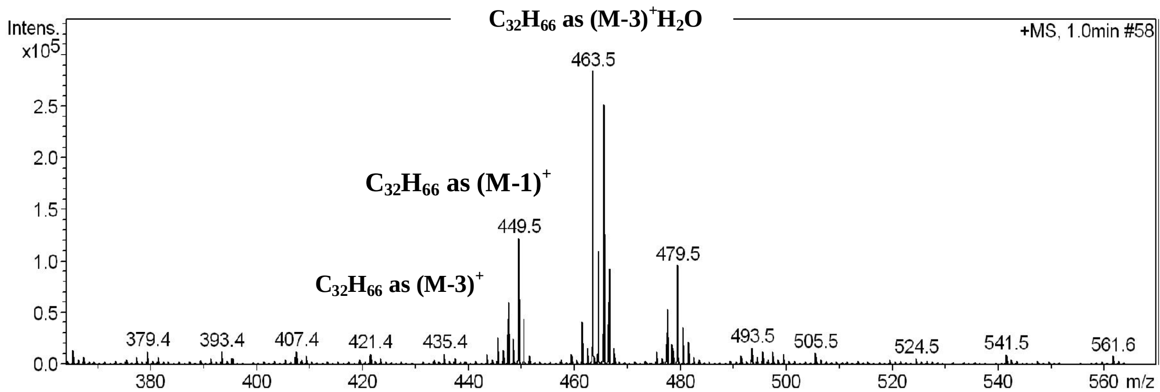
1. Gas chromatograph of hydrocarbons in Light Shredder Waste sample



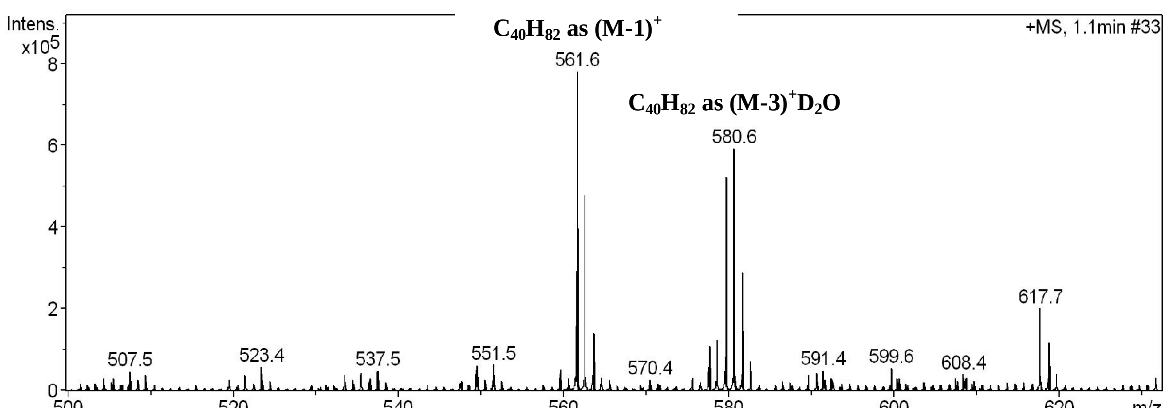
2. Detection of Lower and higher individual *n*-alkanes



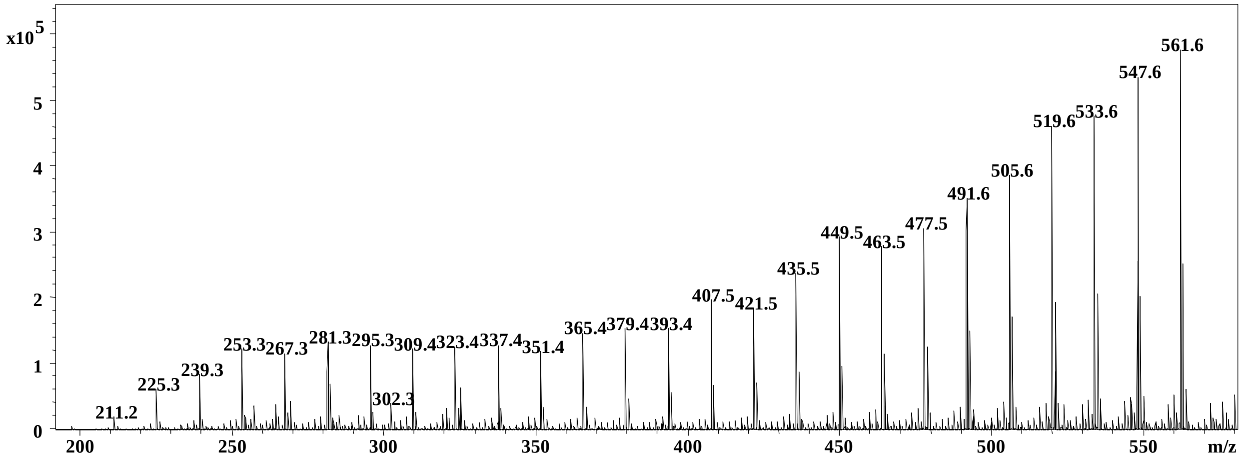




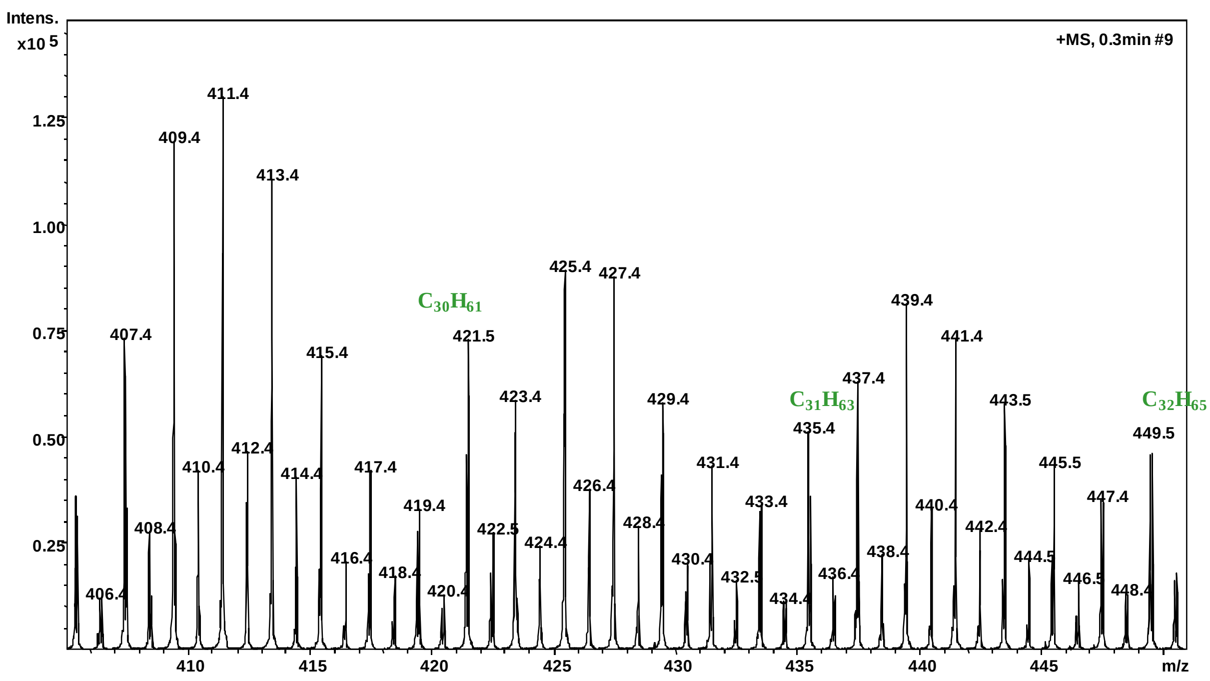
<u>For D2O addition experiment for *n*-tetracontane</u>



3. C7-C40 reference standard at higher concentration

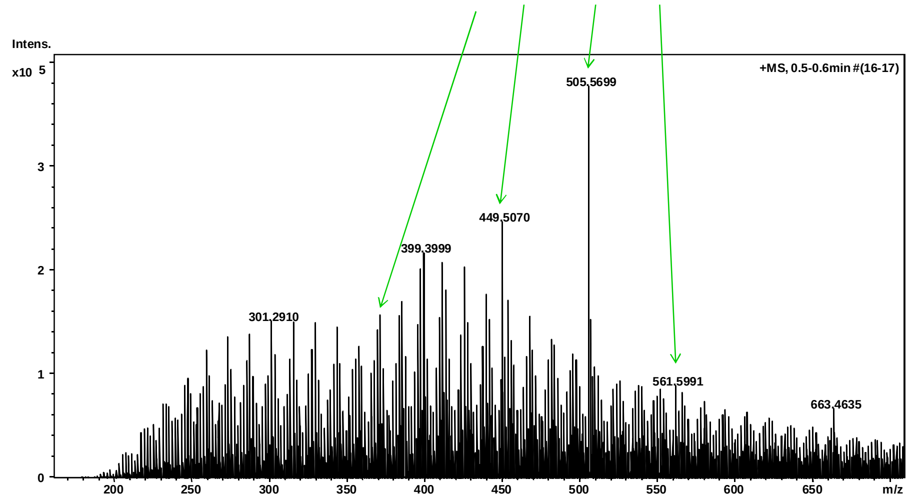


4. Assignment of Mol.Formulas of other *n*-alkanes



5. Spiked higher n-alkane standards into the waste sample

Waste W3 + (C_{26}-C_{32}--C_{36}-C_{40})

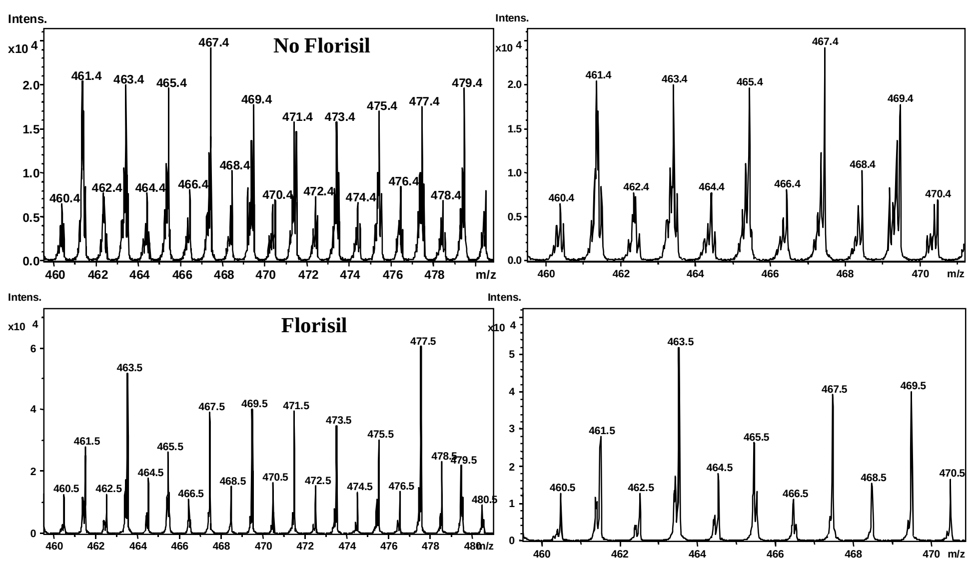


Alkanes are apparently not being suppressed by the other compounds

Alkanes showed promising direct response (Conc vs I)

6. Florisil purification screened in TOF-MS

Florisil Effect



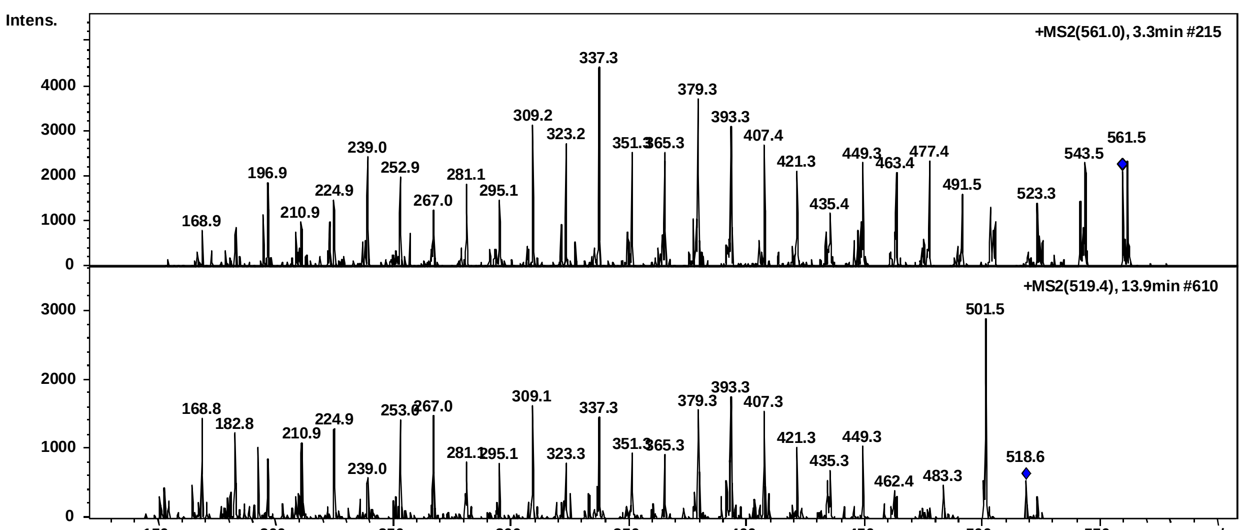
Electronic Supplementary Material (ESI) for Analytical Methods

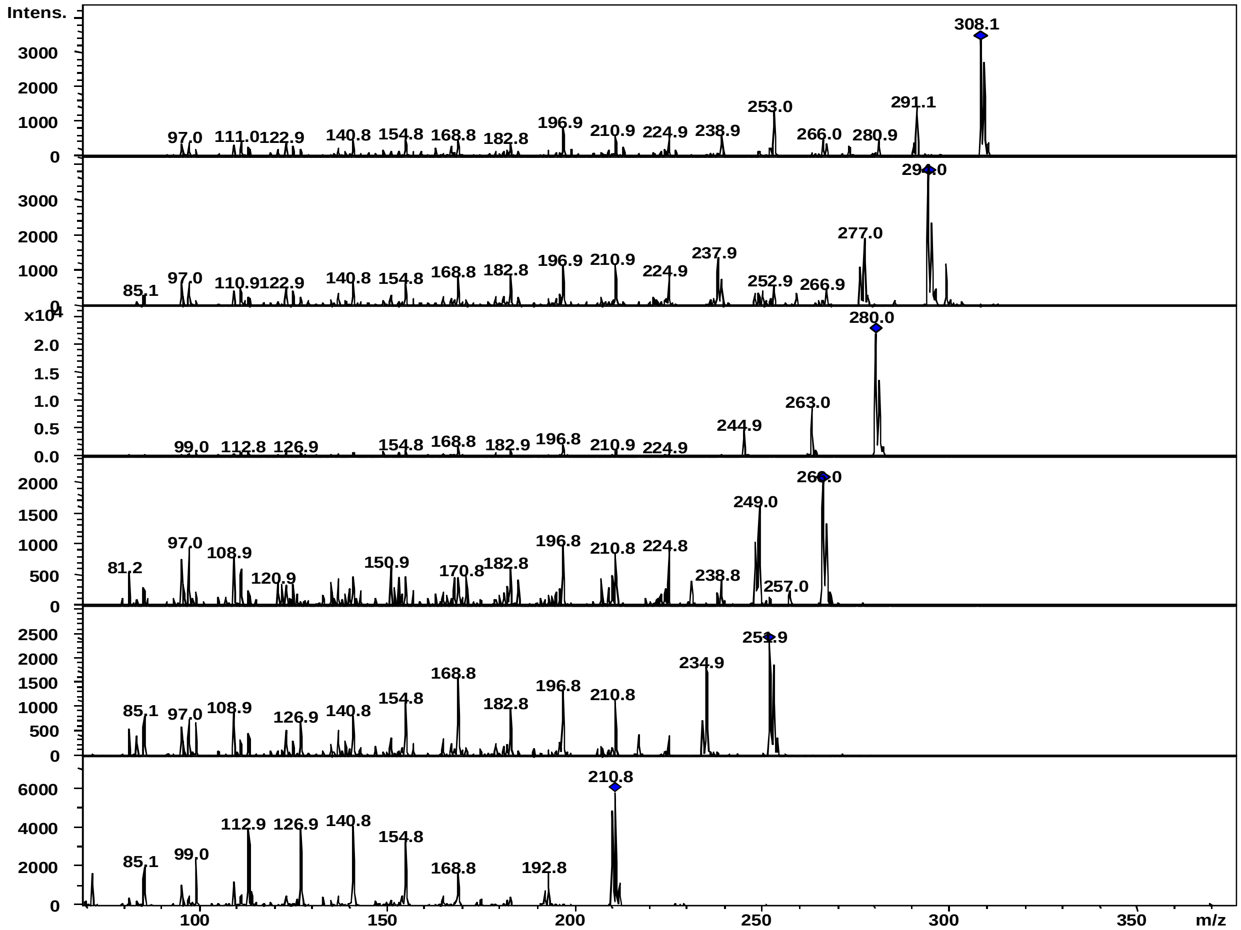
7. Assignment of sample degraded compounds (Dehydrogenation Process reflecting the unsaturated components)

Smart formula list of all compounds in the waste sample

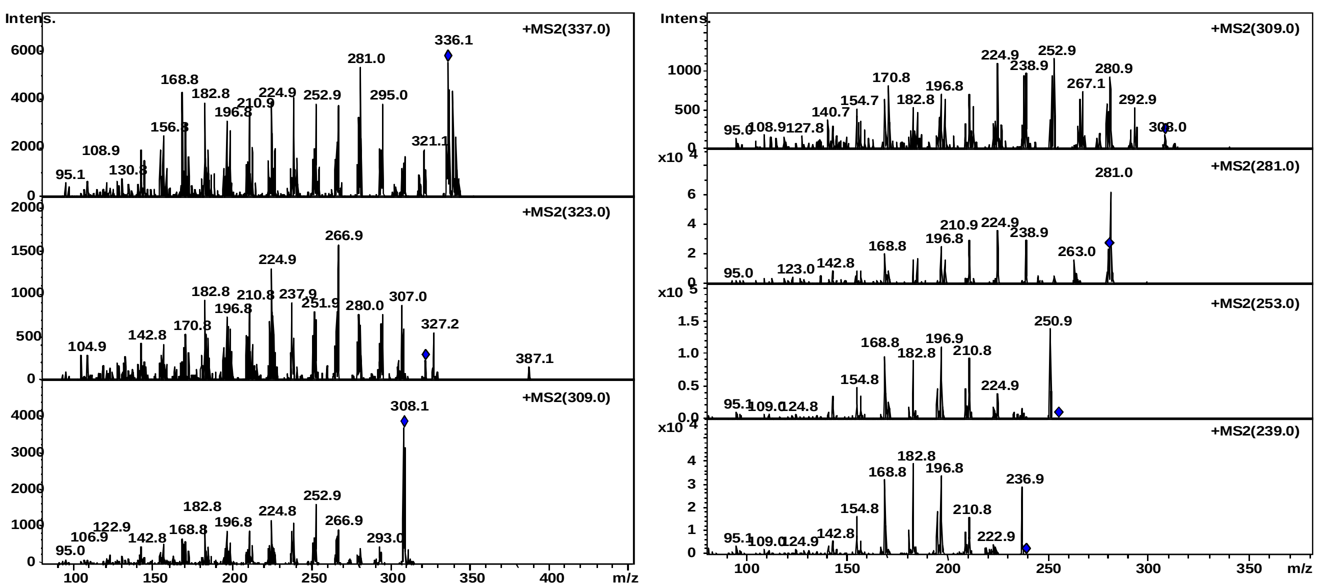
Meas. m/z	Formula	m/z	err [ppm]
189.163	C 14 H 21	189.1638	*4.2*
191.1789	C 14 H 23	191.1794	*2.9*
193.1941	C 14 H 25	193.1951	*5.2*
195.2105	C 14 H 27	195.2107	*1.4*
197.2259	C 14 H 29	197.2264	*2.3*
199.1477	C 15 H 19	199.1481	*2*
201.164	C 15 H 21	201.1638	*-1.2*
203.1796	C 15 H 23	203.1794	*-0.9*
205.1954	C 15 H 25	205.1951	*-1.8*
207.211	C 15 H 27	207.2107	*-1.5*
209.2266	C 15 H 29	209.2264	*-1*
211.2422	C 15 H 31	211.242	*-1*
213.1647	C 16 H 21	213.1638	*-4.5*
215.1804	C 16 H 23	215.1794	*-4.4*
217.1956	C 16 H 25	217.1951	*-2.6*
219.2109	C 16 H 27	219.2107	*-0.6*
221.2274	C 16 H 29	221.2264	*-4.5*
223.2427	C 16 H 31	223.242	*-2.8*
225.2586	C 16 H 33	225.2577	*-4.3*
231.212	C 17 H 27	231.2107	*-5.5*
233.2273	C 17 H 29	233.2264	*-4*
235.2429	C 17 H 31	235.242	*-3.6*
237.258	C 17 H 33	237.2577	*-1.5*
239.274	C 17 H 35	239.2733	*-3*
241.1965	C 18 H 25	241.1951	*-5.9*
245.2276	C 18 H 29	245.2264	*-5.2*
247.2432	C 18 H 31	247.242	*-4.6*
249.2591	C 18 H 33	249.2577	*-5.8*
251.274	C 18 H 35	251.2733	*-2.8*
253.2904	C 18 H 37	253.289	*-5.5*
261.2592	C 19 H 33	261.2577	*-5.7*
263.2747	C 19 H 35	263.2733	*-5.2*
265.2884	C 19 H 37	265.289	*2*
267.3051	C 19 H 39	267.3046	*-1.9*
279.3057	C 20 H 39	279.3046	*-4*
281.3214	C 20 H 41	281.3203	*-3.9*
289.2906	C 21 H 37	289.289	*-5.5*
291.306	C 21 H 39	291.3046	*-4.7*
293.3212	C 21 H 41	293.3203	*-3.3*
295.3374	C 21 H 43	295.3359	*-5.1*
303.3062	C 22 H 39	303.3046	*-5.3*
305.3215	C 22 H 41	305.3203	*-4.1*
307.3367	C 22 H 43	307.3359	*-2.7*
309.3522	C 22 H 45	309.3516	*-2*
317.3219	C 23 H 41	317.3203	*-5.1*
319.3375	C 23 H 43	319.3359	*-4.8*
321.3515	C 23 H 45	321.3516	*0.2*
323.3685	C 23 H 47	323.3672	*-3.9*

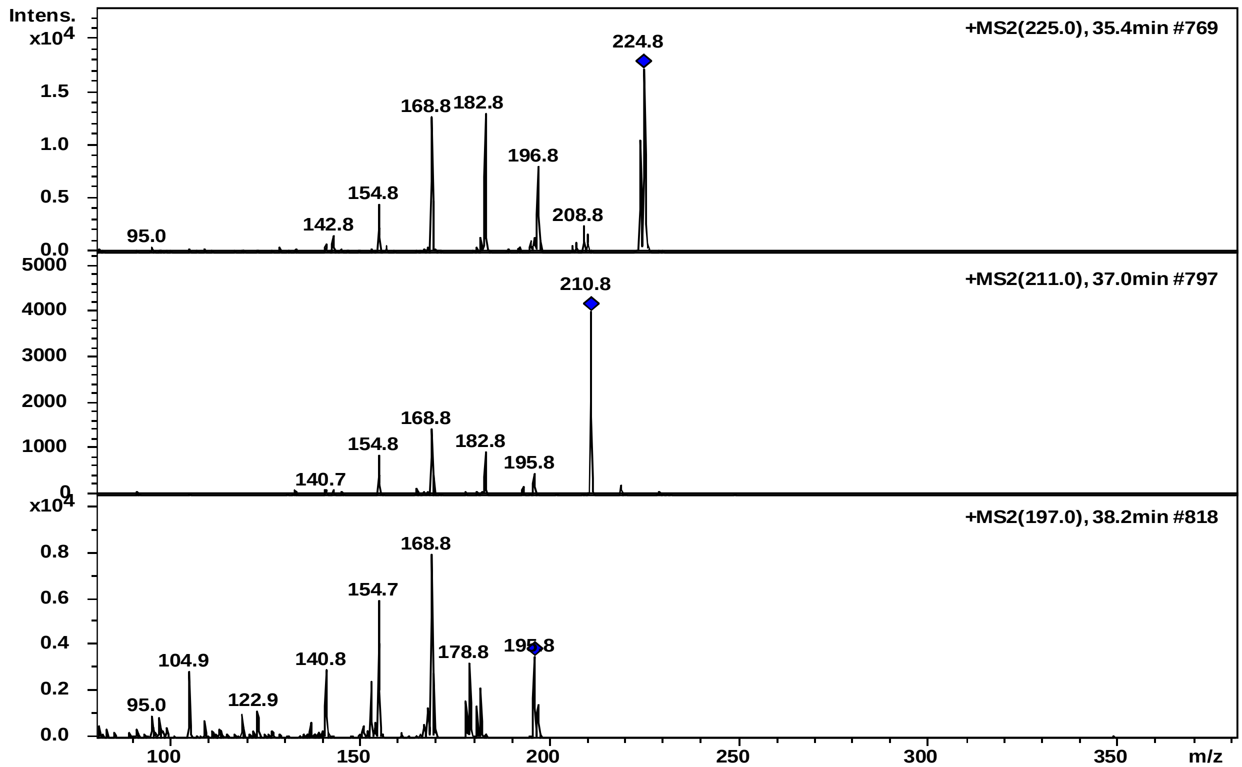
8. Fragmentation pattern of *n*-alkanes in standard mixtures



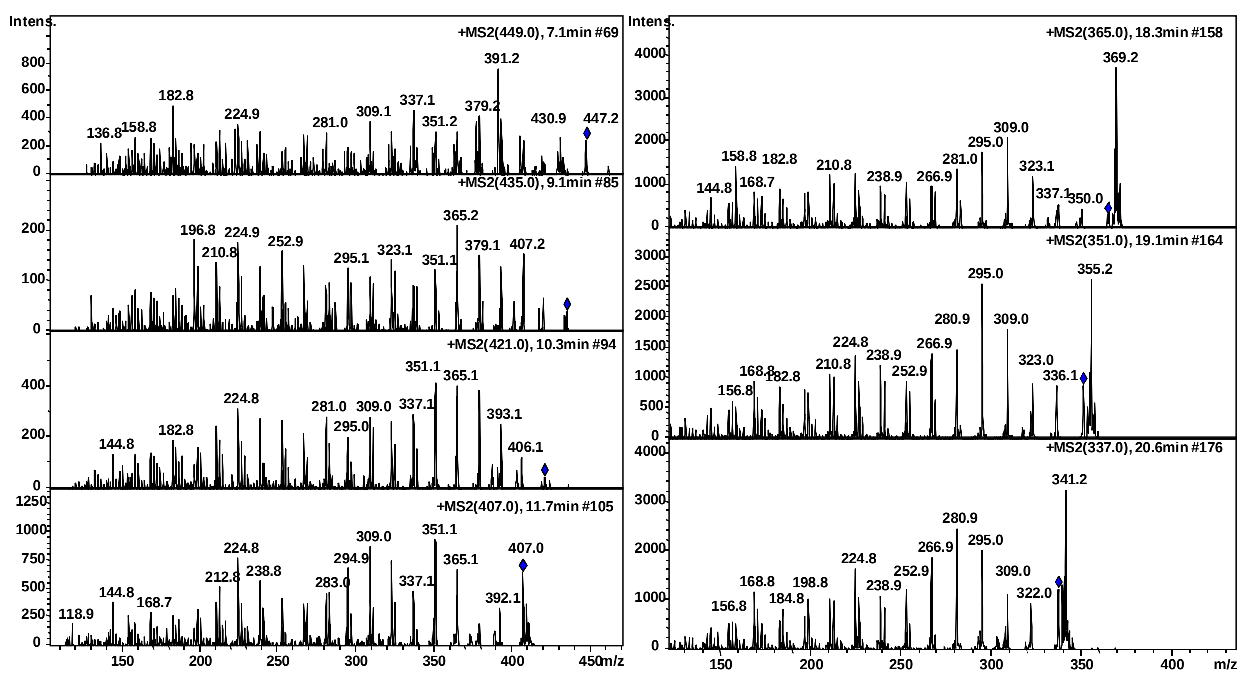


9. Fragmentation pattern of *n*-alkanes within waste sample W1





Alkane within another waste sample W2 : **Fragmentation yielding identical MS2 patterns which are similar to the pattern associated to the reference standards of n-alkanes**



10. Calibration curves (0.2 ppm to 40 ppm) *vs* I